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Adsorption of Sr from waste effluents using Taiwan Zhi-Shin bentonite

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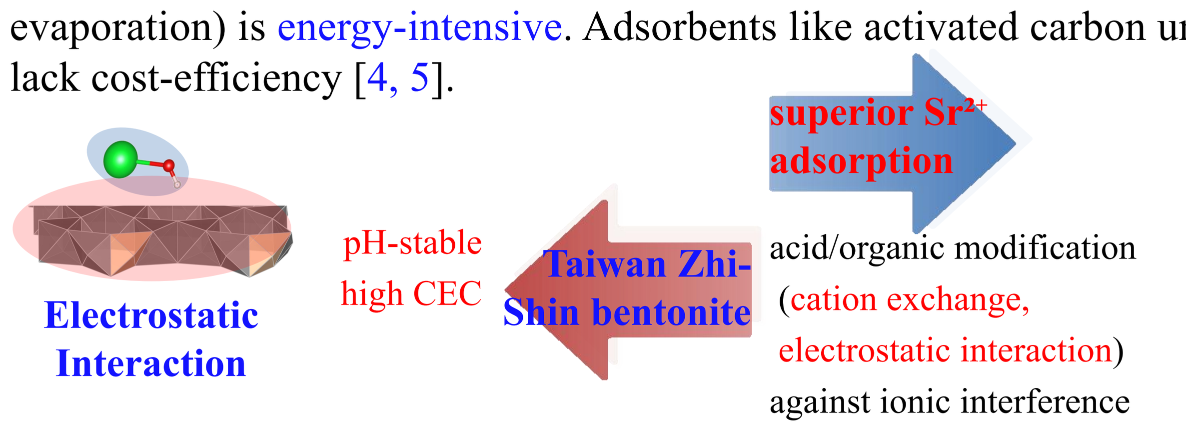
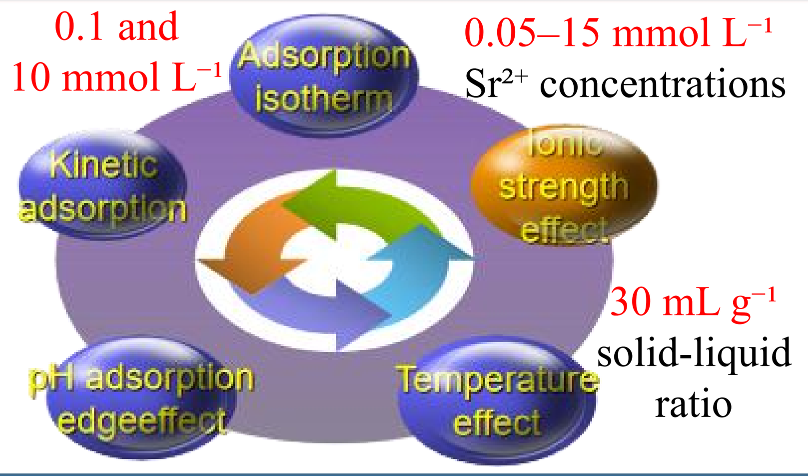
INTRODUCTION

Strontium-90 (28.79-yr half-life), a bone-accumulating radionuclide linked to leukemia [1], contaminates aquatic systems (e.g., post-Fukushima) [2]. Conventional removal (ionic exchange, evaporation) is energy-intensive. Adsorbents like activated carbon underperform [3]; MOFs/hydrogels lack cost-efficiency [4, 5].



Objective
- Batch experiments: Sr^{2+} adsorption under varied factors.
- XRD/simulations: pH/concentration-dependent **cation exchange** dominant.

METHOD



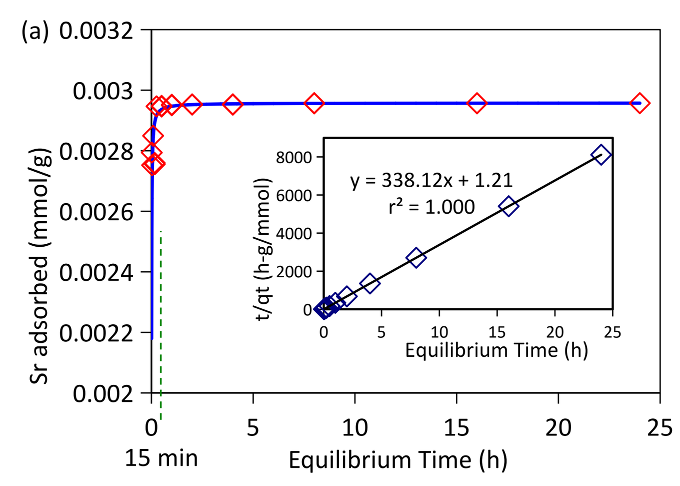
Molecular simulation verifies the adsorption mechanism

A cell model with a size of 2a × 1b × 1c (17.96Å × 10.36Å × 39.00Å) Interaction in bentonite supercells, and the adsorption mechanism was verified by AIMD.

RESULTS & DISCUSSION

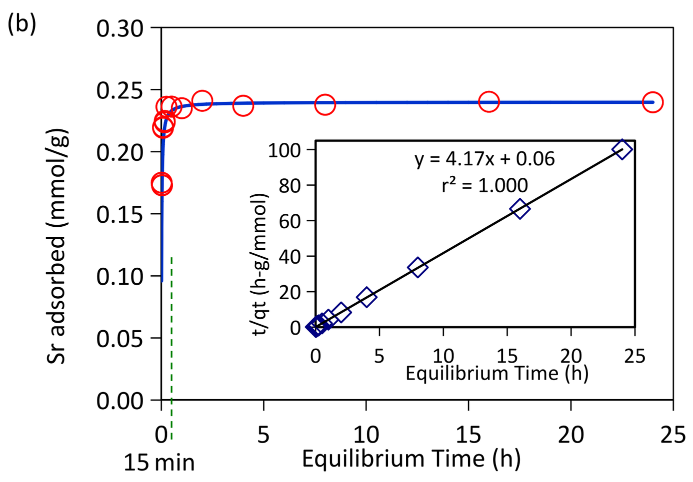
3.1 Adsorption kinetics experiment of Sr^{2+}

95% Sr^{2+} removed in 5 min (**15 min** equilibrium, 0.1-10 mM) via cation exchange (pseudo-second-order, r^2=1.000)(Fig. 1a, b). outperforms MOFs/zeolites in cost-effective [4, 6].



3.2 Adsorption isotherm experiment of Sr^{2+}

Sr^{2+} isotherm on Taiwan Zhi-Shin bentonite fits **Freundlich** (r^2=0.96), 24.53 mg g^{-1} (**65–70% CEC**) (Fig. 1c). Outperforms engineered materials (Na-bentonite, MOFs) via natural abundance, no pretreatment, cost-efficiency [4, 7]; unmodified Ca-bentonite suits nuclear waste.



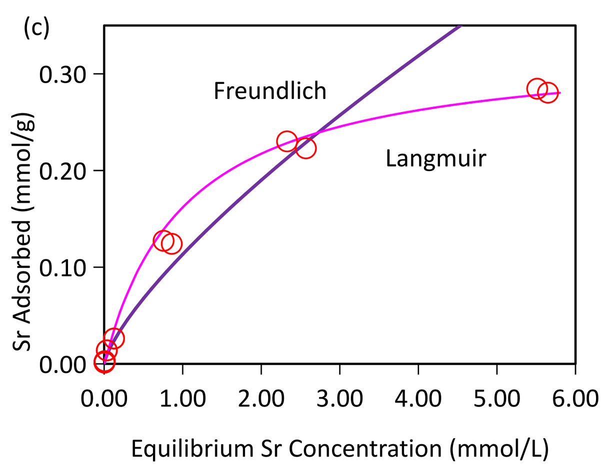
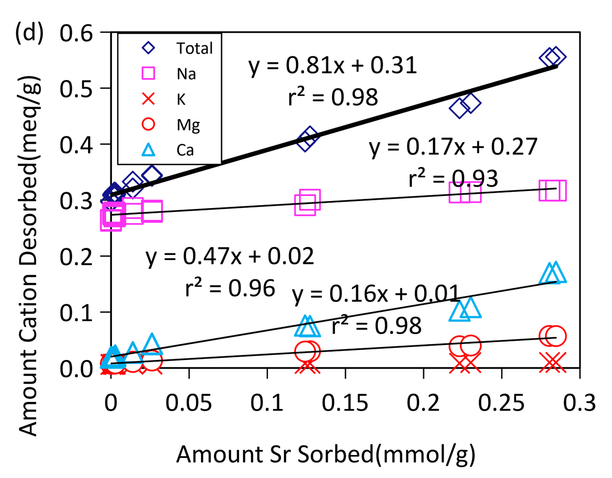


Fig. 1a-b: Sr^{2+} sorption kinetics (0.1/10 mM) on Taiwan Zhi-Shin bentonite, pseudo-second-order fit (solid lines) with linear insets. 1c: Langmuir/Freundlich isotherms. 1d: Cation desorption vs Sr^{2+} adsorption. 1e: Temperature-dependent adsorption (0.1/10 mM-Sr) with thermodynamics.



3.3 Experiments on influencing factors of adsorption of Sr^{2+}

3.3.1 Exchangeable cation desorption

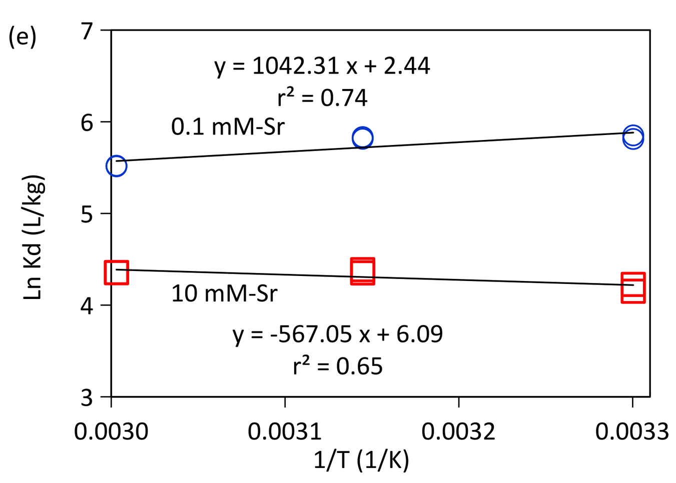
Taiwan Zhi-Shin bentonite: Sr^{2+} adsorption via **cation exchange** (**Ca^{2+} 60.4% released**; Na^+/Mg^{2+} minimal, K^+ negligible; Fig. 1d). Sr^{2+}-cation correlation confirms interlayer exchange [8].

3.3.2 Effect of temperature on Sr^{2+} adsorption

Fig. 1e: 0.1 mM Sr^{2+}: exothermic (ΔH<0, ΔG=-6.1 kJ mol^{-1}), entropy loss (ΔS=-0.01), spontaneous but temperature-inhibited. 10 mM: endothermic (ΔH=+4.71), entropy gain (ΔS=+0.02), temperature-enhanced via dehydration/steric effects.

3.3.3 Influence of pH value

Taiwan Zhi-Shin bentonite: pH-dependent Sr^{2+} adsorption (**optimal >9**). 0.1 mM: rapid saturation via **surface electrostatics** (Fig. 2a); 10 mM: **Na^+/Ca^{2+} competition** until pH>9 (Ca^{2+} precipitation, $Sr(OH)^+$ generation) (Fig. 2b)[9,10]. Dynamics: Sr^{2+} hydrolysis, cation competition, PZC (9.2) regulates sites.



3.3.4 Effect of ionic strength on adsorption

Ionic strength tests confirm cation exchange dominates Sr^{2+} adsorption (Fig. 2c, d): NaCl (0.01–1 mM) reduces uptake (0.21→0.04 mmol g^{-1} at 10 mM-Sr), consistent with clays [11].

Ci	pH	Ln(Kd)(L/Kg)			△G°(kJ/mol)			△H°(kJ/mol)	△S°(KJ/mol K)
		303K	318K	333K	303K	318K	333K		
0.1mM	9	2.43086	2.42254	2.11603	-0.62492	-6.1295	-6.0099	-8.67	-0.01
10mM	9	0.78774	0.96798	0.9534	-2.06	-2.93	-2.73	4.71	0.02

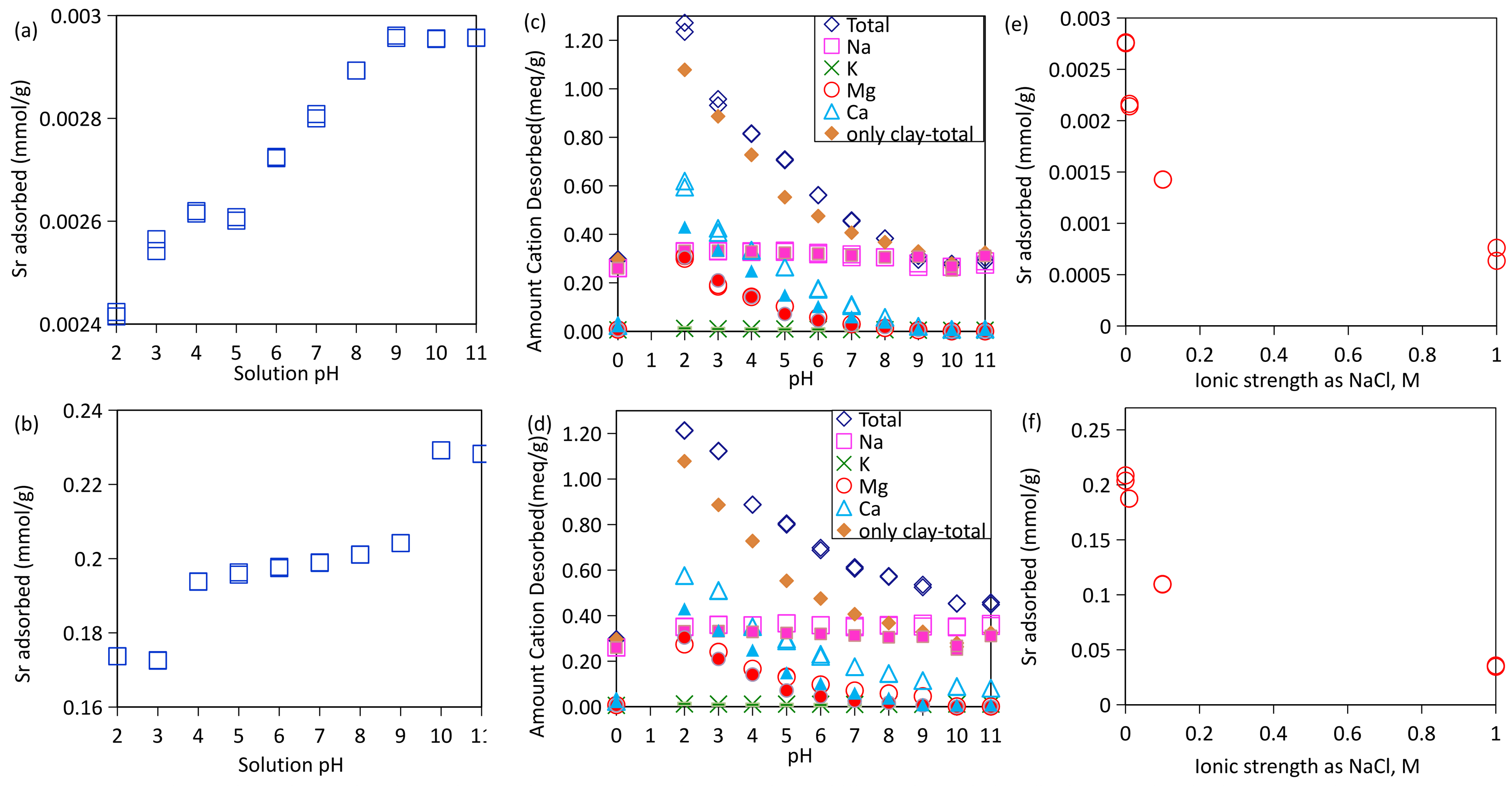
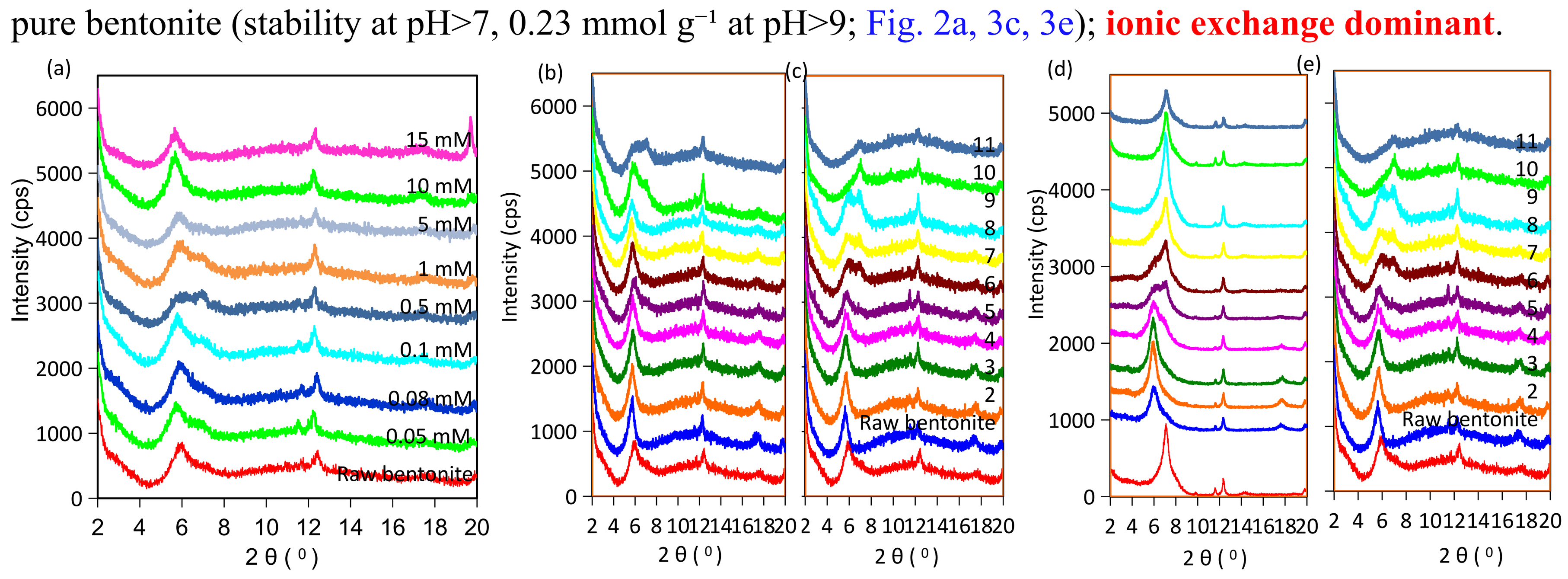


Fig. 2a-b: pH-dependent cation desorption (0.1/10 mM-Sr). 2c-d: Adsorption stability under varied pH/ionic strength at both concentrations. 2e-f: Ionic strength effects on Sr^{2+} adsorption.

3.4 XRD

Taiwan Zhi-Shin bentonite: Sr^{2+} adsorption via montmorillonite interlayer exchange (Sr^{2+} replaces Ca^{2+} with hydrated molecules, (001) 14.71→15.6 Å at pH=9; Fig. 3a)[12,13]. Kaolinite synergizes ((001) 7.1→7.23 Å; [14,15]). Low Sr^{2+} (0.05–5 mM): interstratified hydration (15.5/12.5 Å, competitive exchange; Fig. 3a)[16,17]; high (10–15 mM)/alkaline: uniform 15.6 Å expansion[18,19]. pH: <7 limits hydration (d001≈15.0 Å); >7 enhances intercalation (≈15.6 Å); >10 re-stratifies (Fig. 3b). Outperforms pure bentonite (stability at pH>7, 0.23 mmol g^{-1} at pH>9; Fig. 2a, 3c, 3e); **ionic exchange dominant**.



3.5 Molecular simulation

AIMD: Sr^{2+} adsorption on Ca-bentonite via **H-bonds** (hydration water bridges Sr^{2+}/Ca^{2+} to surface O) and **water bridges** (Fig. 3f-g), strengthened by interlayer hydration. Adsorption energies (−16.08 eV Sr^{2+} vs. −15.55 eV Ca^{2+}) and DFT (−15.30 eV Sr^{2+}) show stronger Sr^{2+} interaction than Na^+ (−7.1 eV). Na-bentonite: H-bonds + ionic exchange. Cation-dependent mechanisms: Ca-bentonite (hydration-mediated), Na-bentonite (competitive adsorption).

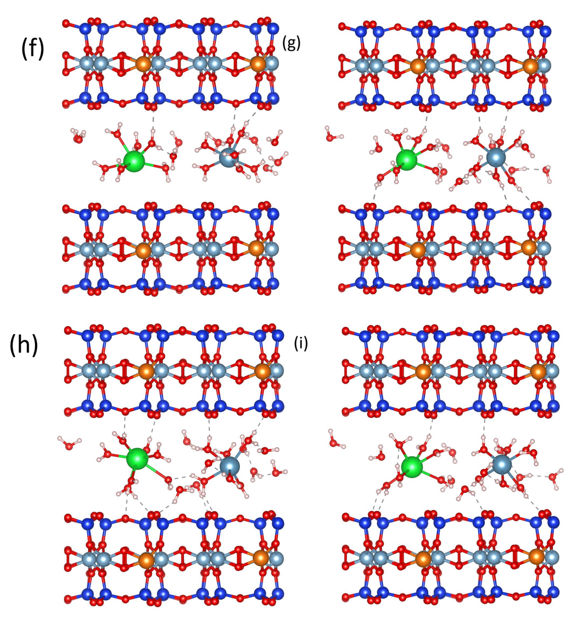
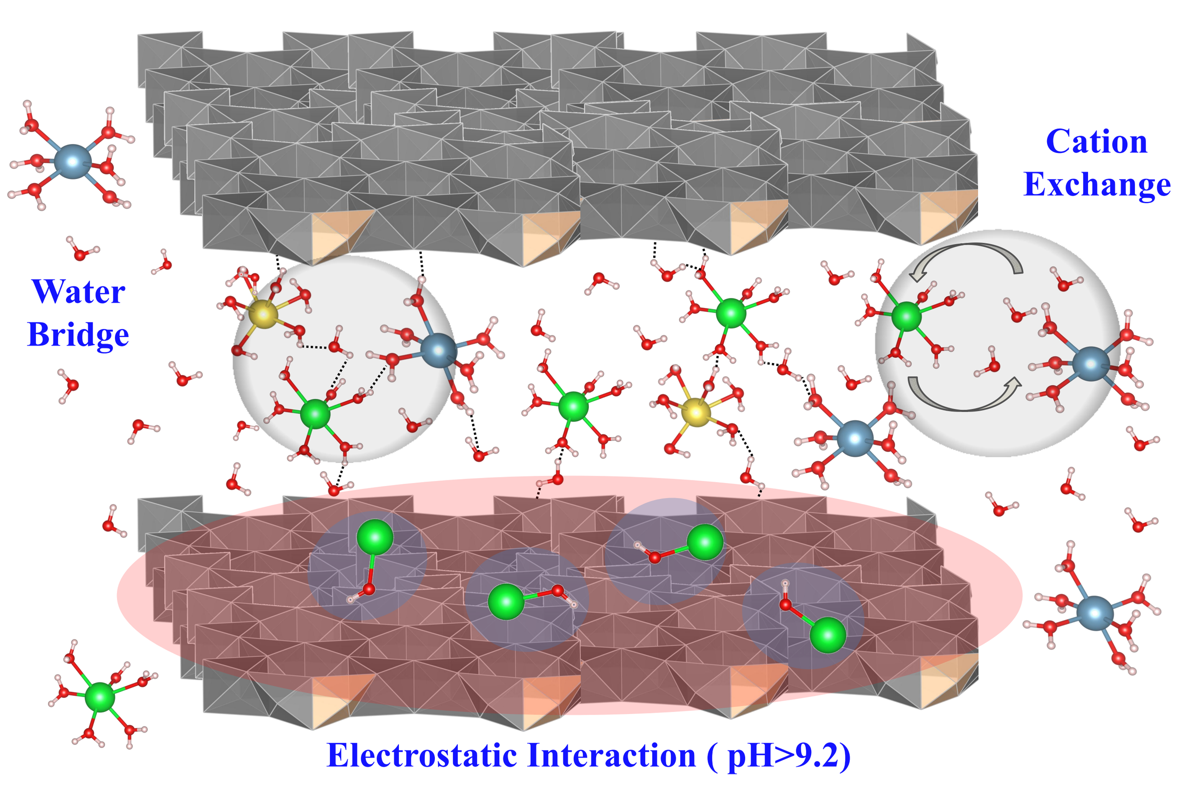


Fig. 3a: XRD of raw and Sr-adsorbed bentonite (0.05-15 mM Sr); 3b: 0.1 mM-Sr adsorption at different pHs; 3c: Bentonite-only XRD (0.1 mM-Sr); 3d: 10 mM-Sr adsorption at different pHs; 3e: Bentonite-only XRD (10 mM-Sr); 3f: Initial Sr^{2+} configuration in Ca^{2+}-bentonite; 3g: AIMD H-bonds (water-surface); 3h: H-bonds/water bridges (Sr^{2+}-Ca^{2+}); 3i: Ca^{2+}-surface water bridge.

CONCLUSION



- Taiwan bentonite achieves **65–70% CEC** utilization for Sr^{2+} adsorption
- Taiwan bentonite achieves **95%** Sr2+ adsorption within **5 minutes** (0.1–10 mM)
- Sr^{2+} forms **H-bond water bridges** on Taiwan bentonite via AIMD simulations
- **Cation exchange** is the main mechanism of Taiwan bentonite
- Taiwan bentonite: **Abundant green** adsorbent for Sr^{2+} removal

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